# Three Month Report

Christopher Baker BSc(Hons)
Imperial College of Science, Technology and Medicine, London

With Thanks to
Prof C.Pain (Supervisor),
Prof A.Goddard (Supervisor),
Dr M.Eaton and Dr A.Buchan

June 12, 2007

# Contents



# List of Figures

# 1 Introduction

This research is focused on the multigroup discretisation of the Boltzmann Transport Equation. The multigroup discretisation is then to be programmed into Imperial College's in-house transport code, RADIANT (RADIAtion Non-oscillatory Transport). This discretisation involves the separation of energy into discrete points, then inputing the group to group scattering and finally entering the fission calculations and eigenvalue calculations. The eigenvalue problem in the fission is calculated using the *power method* Finally, this report has a summary of *dosimetry* which describes the effects of nuclear radiation upon objects, and in particular, humans. The process of dosimetry and the calculations arising are used extensively within medicine.

## 2 The Boltzmann Neutron Transport Equation

My first task was to research in to the multigroup equations and learn the various discretisation methods used using the main transport code, RADIANT. The main discretisation methods used at streamline upwind Petrov - Galerkin (SUPG) methods which can find solutions to a variaty of problems in radiation and in fluid dynamics. My main reference for this report, and much of my work so far is contained in (1) The most important equation in my study is the Boltzmann Neutron Transport Equation, which is defined as follows:

$$\frac{1}{v}\frac{\partial}{\partial t}\psi\left(\vec{r},\hat{\Omega},E,t\right) + \left[\hat{\Omega}\cdot\vec{\nabla}+\sigma\left(\vec{r},E\right)\right]\psi\left(\vec{r},\hat{\Omega},E,t\right) = q\left(\vec{r},\hat{\Omega},E,t\right) \quad (1)$$

over the seven independent variables, space $\vec{r} = (x, y, z)$, angle $\Omega = (\omega, \mu)$ where $cos\chi = \mu$, energy $E$ and time $t$ and $v$ is the speed of the particle. The source $q$ is defined as follows:

$$q\left(\vec{r},\hat{\Omega},E,t\right) = q_{ex}\left(\vec{r},\hat{\Omega},E,t\right) + q_s\left(\vec{r},\hat{\Omega},E,t\right) + q_f\left(\vec{r},\hat{\Omega},E,t\right) \quad (2)$$

which are the external source, scattering source and fission source respectively.
The solution of the equation is then obtained using the discretisation methods of Spherical Harmonics and then SStreamline-Upwind Petrov Galerkin (SUPG) methods.
Firstly, we form the angular discretised form of the Boltzmann equation,

$$\frac{1}{v}\mathbf{A}_t\frac{\partial\boldsymbol{\psi}\left(\vec{r},t\right)}{\partial t} + \mathbf{A}\cdot\vec{\nabla}\boldsymbol{\psi}\left(\vec{r},t\right) + \boldsymbol{\mathcal{H}}\left(\vec{r},t\right)\boldsymbol{\psi}\left(\vec{r},t\right) - \mathbf{s}\left(\vec{r},t\right) = \mathbf{0} \quad (3)$$

where $\mathbf{A} = (\mathbf{A}_x, \mathbf{A}_y, \mathbf{A}_z)^T$, $\boldsymbol{\psi}\left(\vec{r},t\right)$ is a vector of the $\mathcal{M}$ angular moments and $\mathcal{H}$ is a $\mathcal{M}\times\mathcal{M}$ matrix which defines the interaction of the radiation with the host media. The angular moments are calculated from spherical harmonic basis functions, $(Y^e_{lm}, Y^o_{lm})$. The real-valued Spherical harmonics, $Y_{lm}(\hat{\Omega})$, are defined as follows:

$$\begin{array}{l} Y^e_{lm}(\hat{\Omega}) = \frac{(2l+1)(l-m)!}{(l+m)}P^m_l(\mu)\cos(m\omega) \\ Y^o_{lm}(\hat{\Omega}) = \frac{(2l+1)(l-m)!}{(l+m)}P^m_l(\mu)\sin(m\omega) \end{array} \quad (4)$$

where $\mu \equiv \cos\theta$, and where $m \in 0, 1, \ldots, m$, and $l \in 1, \ldots, \infty$, and where $P^m_l$ are the *associated Legendre Polynomials* given by:

$$P^m_l(\mu) = (-1)^m(1-\mu^2)^{m/2}\frac{d^m}{d\mu^m}P_l(\mu) \quad (5)$$

and $P_l$ the *Legendre Polynomials* which satisfy the solutions to the differential equation

$$(\mu^2-1)\frac{d}{d\mu}P)_l = l\left[\mu P_l(\mu) - P_{l-1}(\mu)\right] \quad (6)$$

In the 2D case, this discretisation forms a linear equation with $(l+1)(l+2)$ unknowns, one for each moment of the angular flux. Now the matrix $\mathcal{H}$ can be defined for each element in the matrix as:

$$\mathcal{H}_{ij} = \int d\mu \int d\omega G_i(\mu,\omega)G_j(\mu,\omega) - \sum_{l=0}^{\infty}\sigma_{sl}(\vec{r})\alpha^{e,l,m}_j\alpha^{e,l,m}_i + 2\sum_{l=1}^{\infty}\sigma_{sl}(\vec{r})\sum_{m=1}^{l}(\alpha^{e,l,m}_j\alpha^{e,l,m}_i + \alpha^{o,l,m}_j\alpha^{o,l,m}_i) \quad (7)$$

where the functions $G_j(\hat{\Omega})$ are the Galerkin weighting functions, and the constants $\alpha$ are defined as:

$$\begin{array}{l} \alpha_j^{e,l,m} = \int d\Omega G_j(\hat{\Omega}) Y_{lm}^e(\hat{\Omega}) \\ \alpha_j^{o,l,m} = \int d\Omega G_j(\hat{\Omega}) Y_{lm}^o(\hat{\Omega}) \end{array} \tag{8}$$

Using the finite element SUPG formulation of the transport equation, modified by a premultiplication by an SUPG term.
The $\mathcal{M} \times \mathcal{M}$ *angular* matrix $\mathbf{A}_t$ and the three *angular* Jacobian matrices $\mathbf{A}_x$, $\mathbf{A}_y$ and $\mathbf{A}_z$ are defined by:

$$\mathbf{A}_t = \int g(\Omega) g(\Omega)^T d\Omega \qquad \mathbf{A}_k = g(\Omega)\Omega_k g(\Omega)^T d\Omega \qquad k = x, y, z \tag{9}$$

where $g(\Omega)$ is of size $\mathcal{M}$ and contains the basis functions for the angular expansion, and $\Omega_k$ are the Cartesian components of the particle direction vector in the $k = x, y, z$ direction, so, $\mathbf{\Omega} = (\Omega_x, \Omega_y, \Omega_z)^T = (\sqrt{1-\mu^2} cos\chi, \sqrt{1-\mu^2} sin\chi, \mu)^T$, where $\mu$ is the cosine of the polar angle, and $\chi$ is the azimuthal angle in spherical polar coordinates.

$$\left(\mathbf{I} - \mathbf{A} \cdot \vec{\nabla}\mathbf{P}\right)\left(\frac{1}{v}\frac{\partial \mathbf{\Psi}(\vec{r},t)}{\partial t} + \mathbf{A} \cdot \vec{\nabla}\mathbf{\Psi}(\vec{r},t) + \mathbf{H}(\vec{r})\,\mathbf{\Psi}(\vec{r},t) - \mathbf{S}(\vec{r},t)\right) = \mathbf{0} \tag{10}$$

Then using a Bubnov - Galerkin discretisation method by multiplying the diagonal matrix $N_i(\vec{r})$ an $\mathcal{M} \times \mathcal{M}$ matrix containing the FE basis functions, and integrating over volume and finally applying Green's theorem, we attain:

$$\begin{aligned} -\int_V (\mathbf{A} \cdot \mathbf{N_i}(\vec{r})\,\mathbf{\Psi}(\vec{r},t))\,dV + \int_V \mathbf{N_i}(\vec{r})\left(\frac{1}{v}\frac{\partial \mathbf{\Psi}(\vec{r},t)}{\partial t} + \mathbf{H}(\vec{r})\,\mathbf{\Psi}(\vec{r},t) - \mathbf{S}(\vec{r},t)\right) dV \\ + \int_V \mathbf{A} \cdot \vec{\nabla}\mathbf{N_i}(\vec{r})\,\mathbf{P}\mathcal{R} dV + \int_\Gamma \mathbf{N_i}(\vec{r})\,(\mathbf{A} \cdot \mathbf{n})\,\mathbf{\Psi}(\vec{r},t)\,d\Gamma \\ - \int_\Gamma \mathbf{N_i}(\vec{r})\,(\mathbf{A} \cdot \mathbf{n})\,\mathbf{P}\mathcal{R} d\Gamma = \mathbf{0} \qquad \forall i \in \{1, 2, ..., \mathcal{N}\} \end{aligned} \tag{11}$$

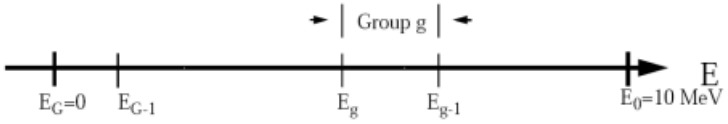
where $\mathbf{n} = (n_x\mathbf{I}, n_y\mathbf{I}, n_z\mathbf{I})^T$ is normal to the boundary $\Gamma$ of the solution domain $V$, $\mathbf{I}$ is the Identity matrix of size $\mathcal{M} \times \mathcal{M}$, $\mathbf{P}$ is the SUPG stablisation matrix, and $\mathcal{R}$ is the equation residual defined by

$$\mathcal{R} = \left(\frac{1}{v}\frac{\partial \mathbf{\Psi}(\vec{r},t)}{\partial t} + \mathbf{A} \cdot \vec{\nabla}\mathbf{\Psi}(\vec{r},t) + \mathbf{H}(\vec{r})\,\mathbf{\Psi}(\vec{r},t) - \mathbf{S}(\vec{r},t)\right) \tag{12}$$

and $\mathbf{\Psi}$, $\mathbf{H}$ and $\mathbf{S}$ are the finite element approximations to the functions $\boldsymbol{\psi}$, $\boldsymbol{\mathcal{H}}$ and $\mathbf{s}$ respectively.

# 3 The Multigroup Equation

To discretise the energy into finite elements, such as below




the formation of the multigroup equations which we can use to solve the Boltzmann Neutron Equation after the discretisation of energy:

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g\left(\vec{r}\right)\right]\psi_g\left(\vec{r},\hat{\Omega}\right)=\sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}\left(\vec{r},\hat{\Omega}'\right)$$
$$+\frac{1}{k}\chi_g\sum_{g'=1}^{G}\upsilon\sigma_{fg'}\left(\vec{r}\right)\phi_{g'}\left(\vec{r}\right) \quad (13)$$

for each group $g \in G$ The functions $\psi_g$ are obtained by integrating over the energy range, so

$$\psi_g\left(\vec{r},\hat{\Omega}\right)=\int_{E_g}^{E_{g-1}}\psi\left(\vec{r},\hat{\Omega},E\right)dE \quad (14)$$

If $f(e)$ is a known function of energy, and the group flux is $\psi_g(\vec{r},\hat{\Omega})$ then this can be made constant,

$$\psi(\vec{r},\hat{\Omega},E)\approx f(E)\psi_g(\vec{r},\hat{\Omega}) \quad (15)$$

where the energy function is normalised to

$$\int_g f(E)dE=\int_{E_g}^{E_{g-1}}f(E)dE=1 \quad (16)$$

and expanding out the $\sigma_{gg'}\left(\vec{r},\hat{\Omega}\cdot\hat{\Omega}'\right)$ term into legendre polynomials as below:

$$\sigma_{gg'}\left(\vec{r},\hat{\Omega}\cdot\hat{\Omega}'\right)=\sum_{l=0}^{\infty}(2l+1)\sigma_{lgg'}(\vec{r})P_l(\Omega\cdot\hat{\Omega}') \quad (17)$$

where

$$\sigma_{lgg'}(\vec{r})=\int_g dE\int_{g'}dE'\sigma_{sl}(\vec{r},E'\rightarrow E)f(E') \quad (18)$$

and expanding the scattering term so that:

$$\sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}\left(\vec{r},\hat{\Omega}'\right)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}^{*}(\hat{\Omega})\sum_{g'=1}^{G}\sigma_{lgg'}(\vec{r})\phi_{lg'}^{m}(\vec{r}) \quad (19)$$

where $\phi_{lg'}^{m}$ are the *legendre moments* of the group flux, defined as

$$\phi_{lg'}^{m}(\vec{r})=\int d\Omega Y_{lm}(\hat{\Omega})\psi_g(\vec{r},\hat{\Omega}) \quad (20)$$

The tolerance level for the convergence for the solutions then has to be decided. This is achieved through a simple convergence tester as below:

$$|\psi_g^i - \psi_g^{i-1}| < \epsilon \tag{21}$$

based on the $i^{th}$ iteration for each group, node and moment. The convergence level has been set to $1 \times 10^{-10}$, with the maximum amount of iterations set to $15$. However, this might this convergence alogorithm might pass the conditions, but in fact has not converged, and so to improve upon this method, a Krylov solver is needed to speed up and check for true convergence of the solution. Krylov solvers can speed up the convergence of the solutions and check if the solution is truely converged. The Krylov solver that will best fit the multigroup convergence is called IVOR, which the single-group solutions are solved with. The basis of Kylov based solvers is to work out the subspace:

$$K_m(A, v) \equiv span(Av, A^2v, A^3v, ...., A^{m-1}v) \tag{22}$$

# 4 Group Scattering

To begin with, I concentrated on only the group scattering, ignoring the fission term, so the equations I was dealing with were

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g\left(\vec{r}\right)\right]\psi_g\left(\vec{r},\hat{\Omega}\right)=\sum_{g'=1}^{G}\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}\left(\vec{r},\hat{\Omega}'\right) \tag{23}$$

for each group $g \in G$
Of which the spherical harmonics discrization is:

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g\left(\vec{r}\right)\right]\psi_g\left(\vec{r},\hat{\Omega}\right)=\sum_{g'=1}^{G}\int d\Omega'\sum_{l=0}^{\infty}\left(2l+1\right)\sigma_{lgg'}\left(\vec{r}\right)P_l\left(\hat{\Omega}'\cdot\hat{\Omega}\right)\psi_{g'}\left(\vec{r},\hat{\Omega}\right) \tag{24}$$

for each group $g \in G$
Now, expanding out the spherical harmonics, and then simplify obtaining:

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g\left(\vec{r}\right)\right]\psi_g\left(\vec{r},\hat{\Omega}\right)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}^{*}\left(\hat{\Omega}\right)\sum_{g'=1}^{G}\sigma_{lgg'}\left(\vec{r}\right)\phi_{lg'}^{m}\left(\vec{r}\right) \tag{25}$$

where the moments of the group flux are defined as

$$\phi_{lg'}^{m}\left(\vec{r}\right)=\int d\Omega Y_{lm}\left(\hat{\Omega}\right)\psi_g\left(\vec{r},\hat{\Omega}\right) \tag{26}$$

The full discretisation of the energy can be obtained by using the streaming operator, as defined below,

$$H_{gg}^{0}\psi_g=\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma_g\left(\vec{r}\right)\right]\psi_g\left(\vec{r},\hat{\Omega}\right) \tag{27}$$

the group to group operator

$$H_{gg'}^{1}\psi_{g'}=\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}\cdot\hat{\Omega}'\right)\psi_{g'}\left(\vec{r},\hat{\Omega}'\right) \tag{28}$$

and finally defining the multigroup operator as

$$H_{gg'}=\delta_{gg'}H_{gg}^{0}-H_{gg}^{1} \tag{29}$$

to form a system of linear equations with $G$ unknowns in the variable $\psi_g$, $(g \in G)$.

$$\begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1g} & \cdots & H_{1G} \\ H_{21} & H_{22} & & & & \\ \vdots & & \ddots & & & \\ H_{g1} & & & H_{gg} & & \\ & & & & \ddots & \\ H_{G1} & & & & & H_{GG} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_g \\ \vdots \\ \psi_G \end{bmatrix} = \begin{bmatrix} q_1^e \\ q_2^e \\ \vdots \\ q_g^e \\ \vdots \\ q_G^e \end{bmatrix} \tag{30}$$

Or more simply

$$\mathbf{H}\boldsymbol{\psi}=\mathbf{q}^{\mathbf{e}} \tag{31}$$

Then this system of equations has to be discretised over space and angle to form the complete discretisation of the phase-space. Now if this is discretised in space and angle, and pre-multiplying the transport equation but an SUPG term, so that

$$\left(\mathbf{I}-\mathbf{A}\cdot\vec{\nabla}\mathbf{P}\right)\left(\mathbf{A}\cdot\vec{\nabla}\boldsymbol{\Psi}_{\boldsymbol{g}}\left(\vec{r}\right)+\mathbf{H}_{\mathbf{g}}\left(\vec{r}\right)\boldsymbol{\Psi}\left(\vec{r}\right)-\mathbf{S}_{\mathbf{g}}\left(\vec{r}\right)\right)=\mathbf{0} \tag{32}$$

Now, after integrating over space and using Green's theorem as in the single-group equations gaining:

$$\begin{aligned}-\int_{V}\left(\mathbf{A}\cdot\mathbf{N}_{\mathbf{i}}\left(\vec{r}\right)\boldsymbol{\Psi}_{\boldsymbol{g}}\left(\vec{r}\right)\right)dV+\int_{V}\mathbf{N}_{\mathbf{i}}\left(\vec{r}\right)\left(\sum_{g'=1}^{G}\mathbf{H}_{\mathbf{gg'}}\left(\vec{r}\right)\boldsymbol{\Psi}\left(\vec{r}\right)-\mathbf{S}_{\mathbf{g'}}\left(\vec{r}\right)\right)dV+\\ \int_{V}\mathbf{A}\cdot\vec{\nabla}\mathbf{N}_{\mathbf{i}}\left(\vec{r}\right)\mathbf{P}\mathcal{R}_{g}dV+\int_{\Gamma}\mathbf{N}_{\mathbf{i}}\left(\vec{r}\right)\left(\mathbf{A}\cdot\mathbf{n}\right)\boldsymbol{\Psi}_{g}\left(\vec{r}\right)d\Gamma\\ -\int_{\Gamma}\mathbf{N}_{\mathbf{i}}\left(\vec{r}\right)\left(\mathbf{A}\cdot\mathbf{n}\right)\mathbf{P}\mathcal{R}_{g}d\Gamma=\mathbf{0}\end{aligned} \tag{33}$$

where

$$\mathcal{R}_{g}=\left(\mathbf{A}\cdot\vec{\nabla}\boldsymbol{\Psi}_{g}\left(\vec{r}\right)+\sum_{g'=1}^{G}\left(\mathbf{H}_{\mathbf{gg'}}\left(\vec{r}\right)\boldsymbol{\Psi}_{g'}\left(\vec{r}\right)-\mathbf{S}_{g'}\left(\vec{r}\right)\right)\right) \tag{34}$$

After the discretisation, a simple way to solve the multigroup equations is to add the scattering terms into the right-hand side of the equation where the sources are kept. $\int d\Omega'\sigma_{gg'}\left(\vec{r},\hat{\Omega}',\cdot\hat{\Omega}\right)\psi_{g'}$ over the groups and adding this to the right hand side vector after the discretisation of space and angle. Due to the orthogonal properties of the spherical harmonics which are used to discretise the angle, when the integal is evaluated, then this simple becomes adding the group to group cross-section to the first element of the right-hand side vector. Some of my test results of the mesh is shown in figure 1 and the solutions obtained in figure 2 which match the results obtained in the older code, EVENT.

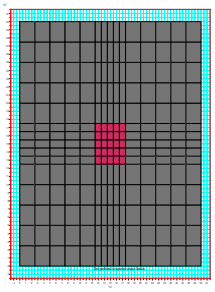
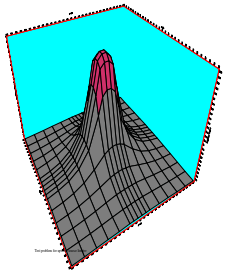
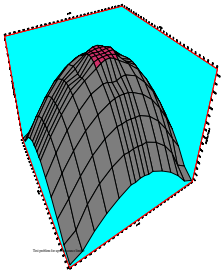


Figure 1: mesh for the problem simple2d-mg

The next problem I solved with the multigroup solver on radiant, is when I changed Radiant to read into upto six groups, and the solutions to the same mesh as before over six energy groups are shown in figure 3 Next, I obtained a problem which is taken from a more realistic problem, using the mesh in figure 4. We obtain the solutions using RADIANT as shown in figure 5.

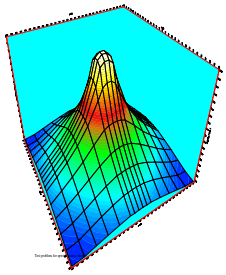


(a) Group 1

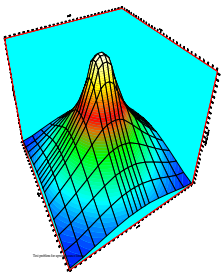


(b) Group 2

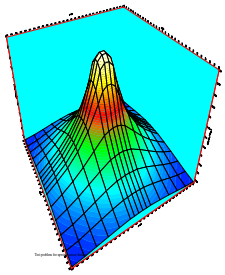
Figure 2: Solutions to the multigroup equations over two groups.



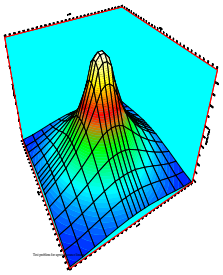
(a) Group 1



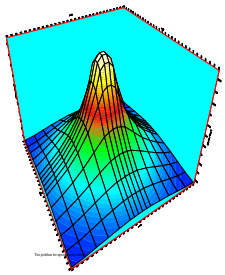
(b) Group 2



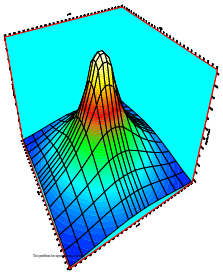
(c) Group 3



(d) Group 4



(e) Group 5



(f) Group 6

Figure 3: The Solutions to the six-group test problem, As you can see from the solutions, the source region is at the peak of the graph showing the scattering of neutrons away from the source, placed in the mesh.

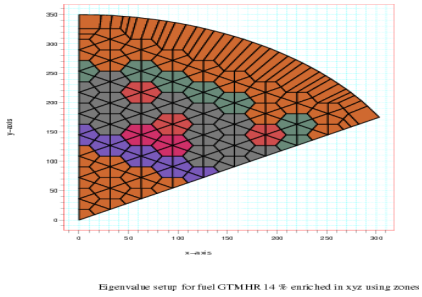
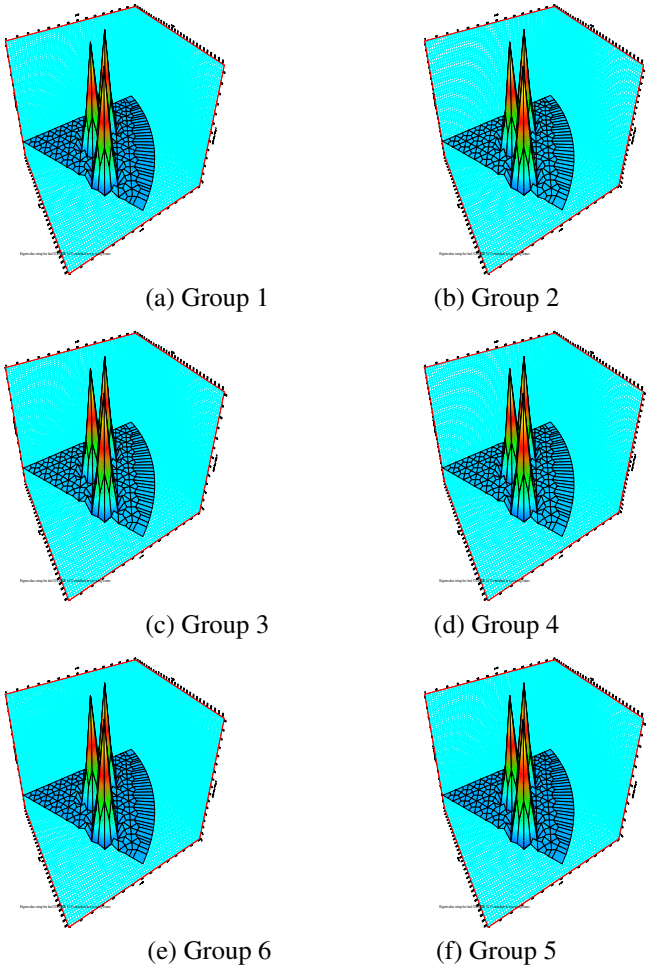



Figure 4: Mesh for real life problem in a reactor



(a) Group 1 (b) Group 2

(c) Group 3 (d) Group 4

(e) Group 6 (f) Group 5

Figure 5: The Solutions to the six-group test problem, As you can see from the solutions, the source region is at the peak of the graph showing the scattering of neutrons away from the source, placed in the mesh.

# 5 Fission

This fission of a multigroup equation is defined as

$$\frac{1}{k}\chi_g \sum_{g'=1}^{G} v\sigma_{fg'}\left(\vec{r}\right)\phi_{g'}\left(\vec{r}\right) \tag{35}$$

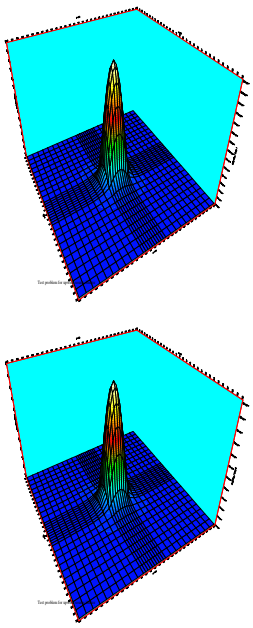
Most of the values needed can be calculated from the nuclear data provided by WIMS, such as $\chi_g$and $v\sigma_{fg'}$, and the *scalar flux*, $\phi_{g'}$ is defined as

$$\phi\left(\vec{r}\right) = \int \psi_{g'}\left(\vec{r},\hat{\Omega}\right) d\Omega \tag{36}$$

$v(E)$ is defined as the mean number of fission neutrons produced in a fission caused by a neuton with energy E, $\chi(E)dE$ is the probability that a fission neutron will have an energy within $dE$ about $E$, and satisfies the properties of a probability distribution function. We can define the probable number of fission neutrons produced at $\vec{r}$ with energies with $dE'$ about $E'$ within the cone of angles $d\Omega$ per path length traveled by neutrons with energy $E$ as

$$v(E)\sigma_f)(\vec{r},E)\chi(E')dE'd\Omega \tag{37}$$

To program the fission term, the fission has to be discretised into space and angle, and this simply yields the same discretisation as the scattering cross-sections, so the fission term can be added onto the scattering cross-sections and to the first moment due to the integration out of angle and the orthongonality of spherical harmonics. After programming the fission terms into Radiant, by the discretisation of angle and space, the results obtained in (fig.6 were obtained for a two group problem which had fission but no external sources in the problem.



(a) Group 1 (b) Group 2

Figure 6: The Solutions to the two-group fission test problem. This shows the fission contributing localised at the centre of the mesh and scattering towards its boundary's.

# 6 Eigenvalue problems and criticality

The k-effective eigenvalue can form time-independent solution by converting $v$, the average number of neutrons per fission to $v/k$ and reform the Neutron Transport Equation to

$$\left[\hat{\Omega}\cdot\vec{\nabla}+\sigma\left(\vec{r},E\right)\right]\psi\left(\vec{r},\hat{\Omega},E\right)=\int dE'\int d\Omega'\sigma_s\left(\vec{r},E'\rightarrow E,\Omega'\cdot\Omega\right)\psi\left(\vec{r},\hat{\Omega}',E'\right)$$
$$+\frac{\chi(E)}{k}\int dE'v\sigma_f\left(\vec{r},E'\right)\int d\Omega'\psi\left(\vec{r},\hat{\Omega}',E'\right) \quad (38)$$

Where $k$ describes the criticality of the system, and the state is defined as

$$k=\begin{cases}>1 & \text{supercritical}\\ =1 & \text{critical}\\ <1 & \text{subcritical}\end{cases}$$

If the system is subcritical then the hypothetical number of neutrons per fission , $v/k$ is larger then the number available in reality, $v$. On the other hand, if the system is supercritical then fewer neutrons per fission are required to make the system critical. We can form the eigenvalue equation by introducing two vectors formed of the $v(E)$ multiplied by the fission cross-sections and the probability distribution function $\chi(E)$, as follows:

$$\mathbf{f}^T=\{v\sigma_{f1}(\vec{r}),v\sigma_{f2}(\vec{r}),\ldots,,v\sigma_{fg}(\vec{r}),\ldots,v\sigma_{fG}(\vec{r})\} \quad (39)$$

and

$$\boldsymbol{\chi}^T=\{\chi_1,\chi_2,\ldots,\chi_g,\ldots,\chi_G\} \quad (40)$$

Then rewriting Eq.(35) in vector form:

$$\sum_{g'}v\sigma_{fg'}(\vec{r})\phi_{g'}(\vec{r})=\mathbf{f}^T(\vec{r})\int\psi(\vec{r},\hat{\Omega})d\Omega \quad (41)$$

and

$$\mathbf{q}_f=\boldsymbol{\chi}\mathbf{f}^T(\vec{r})\int\psi(\vec{r},\hat{\Omega})d\Omega \quad (42)$$

These vectors can then form the basis of the eigenvalue equation:

$$AF=kF \quad (43)$$

by defining the scalar transport operator as

$$A\equiv\mathbf{f}^T\int\mathbf{H}^{-1}\boldsymbol{\chi}d\Omega \quad (44)$$

and the scalar quantity that defines the spatial distribution of fission neutrons produced in the reactor as

$$F(\vec{r})=\mathbf{f}(\vec{r})^T\int\psi(\vec{r},\hat{\Omega})d\Omega \quad (45)$$

One of my problems when researching the fission term was how to calculate the operator $A$. This was due to $A$ not forming a matrix, but being a scalar. The next step

is to compute the eigenvalue $k$. The can be achieved by using the *power method* algorithm to solve eigenvalue problems in linear algebra, such as in (5) and the power method which is most relevant to the neutron transport equation is contained in (2) and outlined as follows:

**Algorithm 1** *Power Algorithm for $K$-effective eigenvalue*

1. *Guess core geometry and composition*
2. *Guess inital fission source $S^{(0)}$ and $k^{(0)}$*
3. $M\phi^{(n+1)} = \frac{1}{k^{(n)}} S^{(n)}$
   $S^{(n+1)} = F\phi^{(n+1)}$
   $k^{(n+1)} = \frac{\int d^3 r S^{(n+1)}(\vec{r})}{\frac{1}{k^{(n)}} \int d^3 r S^{(n)}}$
4. *Convergence test*
   $|\frac{k^{(n)} - k^{(n-1)}}{k^{(n)}}| < \epsilon_1$ *and* $|\frac{S^{(n)} - S^{(n-1)}}{S^{(n)}}| < \epsilon_2$
5. *If (3) has not converged then go back to 2*
6. *If (3) has converged then test*
   $k_{eff} \stackrel{?}{=} 1$
7. *if (6) is true then finish*
8. *if (6) is not true go to (1) (Critically search)*

This algorithm has been implemented into Radiant by utilising the Radiant solver firstly to solve calculate the eigenvalue, then going back to use Radiant to use the eigenvalue in the neutron transport equation, and then solving the Boltzmann Neutron Transport equation including group to group scattering and the fission sources.

# 7 Dosimetry

Part of my research is into shielding and the effects of the radiation within a person. For this, *dosimetry*, the theory of radiation dosages, is useful, especially within medicine. Dosimetry can be used to calculate the effects on absorbed material from a source material, which in the case of medicine is organs. If we let $D$ be the quantity of *Radiation Dose* deposited in the absorber material per gram of the absorber material, and measuring in the unit of radiation dose, the *gray* or Gy, is (7)

$$1\text{Gy} = 1 \text{ joule energy deposited per kg of absorber} \tag{46}$$

and the traditional unit for absorbed dose is the *rad* (Radiation Absorbed Dose) defined as

$$1\text{rad} = 100 \text{ ergs energy deposited per g absorber} \tag{47}$$

Where $1$ rad = $10^{-2}$ Gy = $1$ cGy (as $1$ joule = $10^7$ ergs) We can calculate teh *equivalent dose*, $H$, that describes the damage done to tissue interacting with the radiation. The equivalent dose is measured in the *sievert*. We can calculate the equivalent dose by

$$H = D \times Q \tag{48}$$

Where $D$ is the absorbed dose and $Q$ is the weighting factor depending on the type and energy of the radiation, as follows:

| Type of Radiation | Weighting Factor, $Q$ |
|---|---|
| x rays | 1 |
| $\gamma$ rays | 1 |
| Electrons, Positrons | 1 |
| Neutrons | |
| $<$ 10 keV | 5 |
| 10$-$100 keV | 10 |
| $>$ 100 keV to 2 MeV | 20 |
| 2$-$20 MeV | 10 |
| $>$ 20 MeV | 5 |
| Protons $>$ 2 MeV | 5 |
| $\alpha$ Particles | 20 |

Table 1: Weighting Factors for Different Types of Radiation in the Calculation of Equivalent Dose

The *Cumulated Activity*, $\tilde{A}$ is the product of the amount of activity present in the source and on the length of time for which the activity is present. This is measured in bequerel ·sec (Bq·sec). The cumulated activity is a measurement of the total number of radioactive disintegrations occuring during the time that radioactivity is present at the source. If we let $A(t)$ be the *time-activity curve* that describes the amount of activity in the source region changing with time, then the cumulated activity is calculated by

$$\tilde{A} \approx \int_0^\infty A(t)dt \tag{49}$$

The function $A(t)$ can be complicated and therefore the integral above difficult to analyise. However, if certain assumptions are made, the integral can become easier to evalulate. For example, in medicine, if the uptake by an organ is very rapid with respect to

the half-life of the nuclide, and there is no biological extretion, then the time-activity curve is simply

$$A(t) = A_0 e^{-t \ln 2/T_p} \tag{50}$$

where $T_p$ is the physical half-life of the nuclide, and $A_0$ is the intial activity present, then the cumulated activity is:

$$\tilde{A} \approx A_0 \int_0^\infty e^{-t \ln 2/T_p} dt = \frac{T_p A_0}{\ln 2} \tag{51}$$

This leads to defining the *Equilibruim Absorbed Dose Constant*, $\Delta$ which describes the energy emmited per unit of cumulated energy. This musy be calculated for each type of emmision that occurs from the atom. It is calculated as:

$$\Delta_i = 1.6 \times 10^{-13} N_i E_i \text{ Gy} \cdot \text{kg/Bq} \cdot \text{sec} \tag{52}$$

where $E_i$ is the average energy measured in MeV of the emission $i$ and $N_i$ is the relative frequency of that emmision by the nuclide. We use this constant to work out the *absorbed fraction*,$\phi$ which measures the fraction of the energy emitted by the target. This fraction depends upon the amount of radiation energy reaching the target, and on the volume and composition of the target. This value is determined for each type of emission and the source-target pair in the calculation. We can now calculate the total energy absorbed by:

$$\text{Total energy absorbed (Gy} \cdot \text{kg)} = \tilde{A} \sum_i \phi_i(r_k \leftarrow r_h) \Delta_i \tag{53}$$

where $\phi_i(r_k \leftarrow r_h)$ indicates the absorbed fraction for energy delivered from a source region, $r_h$, to the target $r_k$, and where the sum takes place over all the types of emissions such as neutrons, photons etc and values of $\phi_i(r_k \leftarrow r_h)$ for the source-target pair, and $\tilde{A}$ is the cumulated activity for the source $h$. If the energy absorbed by the target is divided by the mass of the target, $m_t$, then we have the *average absorbed dose*, in grays, to the target from the source, and we have

$$\bar{D}(r_k \leftarrow r_h) = \frac{\tilde{A}}{m_t} \sum_i \phi_i(r_k \leftarrow r_h) \Delta_i \tag{54}$$

Then we can calculate the total dose to the target by summing over all the source regions. Calculating the values of $\phi$ can be quite complex, however, for low energy photons ($\leq$ 10keV) then it can be assumed that the emitted energy is absorbed locally and therefore we can let $\phi = 1$ when the target and the source is the same and $\phi = 0$ otherwise.

# 8 Future Research

The next step is to work on introducing time-dependence into RADIANT, and speeding up the computation of the solution using a Kylov sub-space solver. In the long term, the adjoint form of the Boltzmann Transport Equation will yield interesting results based upon looking at a detector or region affected by radiation, and then using the adjoint version of the equation to effectively working backwards to the source region.

Over the next year, my research will be in the development of discontinuity acceleration methods and space/energy Lanczos solver, and the developement of standard and advanced energy treatments (including step/standard multigroup and space/energy (SUPG) methods. My main area is in the energy discretisation into multigroup equations, and later more advanced methods of discretisation of energy.

I will be working to improve the Kylov solver for the multigroup solutions in Radiant over the next month, and in the next few weeks I will be finishing programming the fission term. In the long term, my research will be be based upon the adjoint transport equation looking into problems where we have an object, such as a person, and working backwards to the source of the neutron streams. In the long term, my research will be the parallelisation of Radiant, developing discretisation methods for energy building upon the standard step of the mulitgroup equatons. Also in my research plan is the development of goal based error metrics for resolving the space/angle mesh. In the second year of my research I will be working on interfacing RADIANT with Rolls-Royce and NEA databank neutron/gamma and covariance data as well GID meshing and MAYAVI and PARAVIEW.

By my next report, I will have researched into

1. Eigenvalue Validation
2. Adjoint method for problems with and without fission
3. Adjoint method for within-energy problems and multigroup problems

And in the longer term,

1. Developing error-based metrics
2. Application of methos to sheilding, radiation damage and core design physics, with benchmarking compared to monte carlo codes.

# References


[1] Computational Methods of Neutron Transport, E.E. Lewis, W.F. Miller, Jr., (1993)

[2] Nuclear Reactor Analysis, J.Duderstadt, L.Hamilton

[3] Space-Time Streamline Upwind Petrov - Galekin Method for the Boltmann Transport Equation, Prof C.Pain et al

[4] Finite Elements and Approximation, O.C. Zienkiewicz and K. Morgan (1983)

[5] An Introduction to Numerical Methods in C++, B.H. Flowers (2000)

[6] Fortran 90 For Scientists and Engineers, B.D. Hahn (1994)

[7] Physics in Nuclear Radiation, 3rd Edition, S.R. Cherry, J.A. Sorenson, M.E. Phelps (2003)